The Bogoliubov Theory of a BEC in Particle Representation

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In the *number-conserving* Bogoliubov theory of BEC the Bogoliubov transformation between quasiparticles and particles is nonlinear. We invert this nonlinear transformation and give general expression for eigenstates of the Bogoliubov Hamiltonian in particle representation. The particle representation unveils structure of a condensate multiparticle wavefunction. We give several examples to illustrate the general formalism.

PACS 03.75.Fi, 05.30.Jp

I. INTRODUCTION

Experimental realization of a Bose-Einstein condensate (BEC) in trapped alkali atoms triggered feverish activity in cold atom physics [1]. Recent development of experimental techniques in trapping and cooling of dilute atomic gases allows for preparation, manipulation and control of a condensate in various states and various trapping potentials. For instance, excitation of a condensate to vortex and solitonic states became possible [2]. Cold atoms are also becoming a convenient toy system to study solid state physics. For example, cold atoms trapped in an optical lattice potential undergo quantum phase transition to Mott insulator phase when the barrier between minima of the lattice potential is increased [3, 4].

Theoretical description of a many body system is a challenge to physicists. At low temperature our understanding of BEC is usually based on a mean field approximation within the Gross-Pitaievskii equation (GPE) [5]. GPE provides satisfactory experimental predictions when depletion of a condensate, induced by interactions between atoms, is negligible. In order to describe these quantum fluctuations around the condensate in a systematic way one can use the Bogoliubov theory of BEC. The key idea of the original Bogoliubov theory [6] is the $U(1)$ symmetry breaking approach where the atomic field operator is assumed to have a nonzero expectation value. This *coherent* state necessarily involves superposition of states with different numbers of atoms, an assumption very far from experimental reality.

A number-conserving Bogoliubov theory has been introduced in [7, 8]. While taking into account a finite number of atoms in a condensate, this theory represents eigenstates of the Bogoliubov Hamiltonian as Fock states with well defined numbers of Bogoliubov quasiparticles in all Bogoliubov modes. In this *quasiparticle* representation it is possible, and even pleasant, to calculate a single particle density matrix. However, higher order correlators are increasingly more painfull to get. For all practical purposes in the quasiparticle representation the multiparticle correlations remain hidden. The single particle density function carries very limited information about a many-body system, as is best illustrated by an example considered by Javanainen and Yoo [9]. They simulated a measurement of atom density distribution in an atomic Fock state $|N, N\rangle$ (it is a model counterpart of an experiment with interference of two separate BECs [10]). With two counter-propagating plane waves as the two modes in the Fock state the single particle density function gives uniform density distribution. However, sampling of the many-body probability density shows that each realization of the experiment reveals an interference pattern. Only after averaging over many realizations one gets the uniform density distribution predicted from the single particle density function.

It seems thus crucial to understand the structure of a condensate multiparticle wavefunction especially when the number of non-condensed atoms becomes considerable and may play a significant role in an outcome of a measurement. In this paper we derive an expression for Bogoliubov eigenstates in *particle* representation i.e. as superpositions over Fock states with well defined numbers of *particles* (atoms) in a condensate and non-condensate single particle states. For example, the state without any quasiparticles (Bogoliubov vacuum) has a pair-correlated form

$$\left(\hat{a}_0^\dagger \hat{a}_0^\dagger + \sum_{m>0} \lambda_m \hat{a}_m^\dagger \hat{a}_m^\dagger\right)^{\frac{N}{2}} |0\rangle \;, \tag{1}$$

where the index m runs over a basis of modes $\phi_m(x)$ orthogonal to the condensate wavefunction $\phi_0(x)$. This pair-correlated ansatz has been proposed in a review by Leggett [11], but (except for a homogeneous condensate [11]) the eigenvalues λ_m and the eigenmodes ϕ_m remain unknown. In this paper we construct a simple relationship between these eigenmodes/eigenvalues and the elementary Bogoliubov excitations of the system for a general inhomogeneous condensate which is of current experimental interest. The pair correlated vacuum state is a foundation on which one can build the theory of BEC entirely in terms of N-particle wavefunctions.

The paper is organized as follows. In Section II we briefly summarize the number-conserving Bogoliubov theory introduced by Castin and Dum [8] for a system with a finite number of particles. In Section III we derive the particle representation of the Bogoliubov eigenstates. In Sections IV,V,VI we illustrate the particle representation with a series of examples: a double well, a triple well, and a condensate in a harmonic potential. We conclude in Section VII.

II. BOGOLIUBOV THEORY WITH A FINITE NUMBER OF PARTICLES

The original Bogoliubov theory (BT) [6] was build around the concept of spontaneous symmetry breaking: the field annihilation operator $\hat{\psi}$ acquires a large nonzero expectation value, $\langle\hat{\psi}(\vec{x})\rangle = \phi_0(\vec{x})$. This nonzero mean is sometimes regarded as a symptom of Bose-Einstein condensation. The original BT is build by expansion in small quantum fluctuations around this large mean, $\hat{\psi}(\vec{x}) = \phi_0(\vec{x}) + \delta\hat{\psi}(\vec{x})$. This method has to be used with a lot of care. For example, careful application of the BT leads to the divergence of the quantum fluctuations that is interpreted as a quantum phase spreading of the condensate [12]. In the original spontaneous symmetry breaking approach the condensate state is not a stationary state because for $\langle\hat{\psi}(\vec{x})\rangle \neq 0$ the number of particles is not well defined and states with different numbers of atoms have different energies. A self-consistent version of the Bogoliubov theory, which explicitly takes into account that there is a well defined number of atoms in a trap, was put forward in Ref. [7] and independently by Castin and Dum [8]. In the present section we briefly summarize the latter results.

In the formalism of Ref. [8] it is assumed that most atoms are condensed, i.e. they occupy the same condensate wavefunction $\phi_0(\vec{x})$. To the leading order the state of the system is a Fock state

$$|\phi_0 : N\rangle \;, \tag{2}$$

with all N atoms in the condensate wavefunction ϕ_0. In this Fock state

$$\langle\phi_0 : N|\; \hat{\psi}\; |\phi_0 : N\rangle = 0 \;, \tag{3}$$

as expected for any state with a well defined number of atoms. Fluctuations around such a perfect condensate are calculated with the help of an expansion

$$\hat{\psi}(\vec{x}) \;=\; \hat{a}_0\; \phi_0(\vec{x}) \;+\; \delta\hat{\psi}(\vec{x}) \;. \tag{4}$$

Here $\hat{a}_0$ annihilates atoms in the condensate wavefunction ϕ_0 while the fluctuation operator $\delta\hat{\psi}$ annihilates in all modes orthogonal to the condensate. To make sure that the ϕ_0 in Eq.(4) is indeed the condensate wavefunction it is further assumed that there is no coherence between the condensed and non-condensed parts,

$$\langle\; \hat{a}_0^\dagger\; \delta\hat{\psi}\; \rangle \;=\; 0 \;. \tag{5}$$

This constraint ensures that ϕ_0 is an eigenstate of the one-body density operator.

Perturbative expansion. — The theory is build by expansion in powers of the "small" $\delta\hat{\psi}$. This operator is "small" when density of depleted (non-condensed) atoms is small as compared to density of the condensate, $\langle\delta\hat{\psi}^\dagger(\vec{x})\delta\hat{\psi}(\vec{x})\rangle \ll N|\phi_0(\vec{x})|^2$.

In dimensionless units a Hamiltonian for N interacting atoms in a trapping potential $V(\vec{x})$ is

$$H = \int d\vec{x}\; \left[\frac{1}{2}\nabla\hat{\psi}^\dagger\nabla\hat{\psi} + V(\vec{x})\hat{\psi}^\dagger\hat{\psi} + \frac{g}{2}\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\right] \;, \tag{6}$$

where g is proportional to the s-wave scattering length. The Hamiltonian (6) is expanded in powers of $\delta\hat{\psi}$.

To zero order in $\delta\hat{\psi}$ the ϕ_0 satisfies a stationary GPE

$$-\frac{1}{2}\nabla^2\phi_0 + V(\vec{x})\phi_0 + Ng_0|\phi_0|^2\phi_0 = \mu\phi_0 \;. \tag{7}$$

For a ϕ_0 that solves the GPE the first order term in the expansion of the Hamiltonian (6) in powers of $\delta\hat{\psi}$ is zero. For small depletion (small number of atoms depleted from the condensate wavefunction) and $N \gg 1$ the second order term can be *approximately* expressed in terms of a number-conserving operator

$$\hat{\Lambda}(\vec{x}) \;=\; \frac{1}{N^{1/2}}\; a_0^\dagger\; \delta\hat{\psi}(\vec{x}) \;. \tag{8}$$

As an example of this approximation take a term

$$\begin{aligned}
&2g\delta\hat{\psi}^\dagger\phi_0^*\hat{a}_0^\dagger\phi_0\hat{a}_0\delta\hat{\psi} = \\
&2gN|\phi_0|^2\frac{\delta\hat{\psi}^\dagger\hat{a}_0^\dagger\hat{a}_0\delta\hat{\psi}}{N} = \\
&2gN|\phi_0|^2\hat{\Lambda}^\dagger\hat{\Lambda} - 2gN|\phi_0|^2\frac{\delta\hat{\psi}^\dagger\delta\hat{\psi}}{N} \approx \\
&2gN|\phi_0|^2\hat{\Lambda}^\dagger\hat{\Lambda} \;.
\end{aligned} \tag{9}$$

The last approximate equality is justified for small depletion.

After all such approximations the second order term in the expansion of the Hamiltonian becomes

$$H_2 \;\approx\; \frac{1}{2}\int d^3\vec{x}\; (\Lambda^\dagger, -\Lambda)\; \mathcal{L}\; \begin{pmatrix} \Lambda \\ \Lambda^\dagger \end{pmatrix}, \tag{10}$$

where

$$\mathcal{L} = \begin{pmatrix} H_{GP} + gN\hat{Q}|\phi_0|^2\hat{Q} & gN\hat{Q}\phi_0^2\hat{Q}^* \\ -gN\hat{Q}^*\phi_0^{*2}\hat{Q} & \left[-H_{GP} - gN\hat{Q}|\phi_0|^2\hat{Q}\right]^* \end{pmatrix}, \tag{11}$$

and

$$H_{GP} = -\frac{1}{2}\nabla^2 + V(\vec{x}) + Ng_0|\phi_0|^2 \;. \tag{12}$$

Here $\hat{Q}$ is a projection operator on the subspace orthogonal to ϕ_0,

$$\hat{Q} \;=\; 1 \;-\; \phi_0\; \langle\phi_0| \;. \tag{13}$$

Bogoliubov modes. — In order to diagonalize $\mathcal{L}$ one can first solve the Bogoliubov-de Gennes equations

$$
\begin{aligned}
&-\frac{1}{2}\nabla^2 U_m + V(\vec{x})U_m + 2g|\phi_0|^2 U_m + g\phi_0^2 V_m = \\
&\mu U_m + \omega_m U_m \ , \qquad (14)\\
&-\frac{1}{2}\nabla^2 V_m + V(\vec{x})V_m + 2g|\phi_0|^2 V_m + g(\phi_0^*)^2 U_m = \\
&\mu V_m - \omega_m V_m \ .
\end{aligned}
$$

The eigenmodes of $\mathcal{L}$ are

$$
u_m \ = \ \hat{Q}\ U_m \quad , \quad v_m \ = \ \hat{Q}\ V_m \ . \qquad (15)
$$

This projection is necessary because the operator $\mathcal{L}$ in Eq.(11) is different from the differential operator in Eq.(14). H_2 is diagonalized by a Bogoliubov transformation

$$
\hat{\Lambda}(\vec{x}) \ = \ \sum_m \ \hat{b}_m \ u_m(\vec{x}) \ + \ \hat{b}_m^\dagger \ v_m^*(\vec{x}) \ . \qquad (16)
$$

Given the normalization conditions

$$
\langle u_m | u_{m'} \rangle \ - \ \langle v_m | v_{m'} \rangle \ = \ \delta_{mm'} \ , \qquad (17)
$$

$\hat{b}_m$'s satisfy bosonic commutation relations

$$
[\hat{b}_m, \hat{b}_{m'}^\dagger] = \delta_{mm'} \ \text{ and } \ [\hat{b}_m, \hat{b}_{m'}] = 0 \ . \qquad (18)
$$

These commutation relations are valid in the present order of the expansion i.e. for small depletion. The $\hat{b}_m^\dagger$ ($\hat{b}_m$) operators create (annihilate) *quasiparticles*. The diagonalized H_2 is a sum over harmonic oscillators

$$
H_{\rm B} \ = \ \sum_m \ \omega_m \ \hat{b}_m^\dagger \hat{b}_m \ . \qquad (19)
$$

Equations (18,19) define the BT in the *quasiparticle* representation.

The Bogoliubov vacuum is an eigenstate of $H_{\rm B}$ without any *quasiparticles*

$$
\hat{b}_m \ |0_b\rangle \ = \ 0 \ , \ \text{for all } m \ . \qquad (20)
$$

In Section III we derive the particle representation of $|0_b\rangle$ state and other Bogoliubov eigenstates (i.e. the states that are a result of action of the creation operators $\hat{b}_m^\dagger$ on the Bogoliubov vacuum).

III. BOGOLIUBOV EIGENSTATES IN PARTICLE REPRESENTATION

For small depletion the approximate Hamiltonian is a sum of harmonic oscillators, see Eq.(19). The eigenstate of the Hamiltonian (19) without any *quasiparticles* is the Bogoliubov vacuum, compare Eq.(20). The formal solution for $|0_b\rangle$ in the *quasiparticle* representation is not suitable for any analysis of the structure of the eigenstate like e.g. comparison with exact diagonalization for model systems. In the following we give an expression for the Bogoliubov eigenstates in the particle representation. It allows one to investigate how atoms are depleted from the condensate wavefunction when strength of interaction between particles increases.

$\hat{b}$'s in terms of a's. — Using the expansion in Eq.(16) and the orthogonality relations in Eq.(17) we can express $\hat{b}$'s in terms of $\hat{\Lambda}$,

$$
\hat{b}_m = \langle u_m | \hat{\Lambda} \rangle - \langle v_m | \hat{\Lambda}^\dagger \rangle \ . \qquad (21)
$$

With definitions

$$
\begin{aligned}
\hat{u}_m \ &\equiv \ \langle u_m | \delta\hat{\psi} \rangle \ , \\
\hat{v}_m^\dagger \ &\equiv \ \langle v_m | \delta\hat{\psi}^\dagger \rangle \ . \qquad (22)
\end{aligned}
$$

and Eq.(8) we get the nonlinear Bogoliubov transformation

$$
\hat{b}_m = \frac{1}{N^{1/2}} \left(\hat{a}_0^\dagger \hat{u}_m - \hat{a}_0 \hat{v}_m^\dagger \right) \ . \qquad (23)
$$

$\hat{a}_0$ annihilates particles in the condensate, while $\hat{u}_m$ and $\hat{v}_m$ annihilate in the modes $u_m(\vec{x})$ and $v_m(\vec{x})$ which by construction are orthogonal to the condensate wavefunction $\phi_0(\vec{x})$.

We note that the right hand side of the Bogoliubov transformation (23) between quasiparticles and particles is nonlinear in particle operators. This nonlinearity is necessary to conserve the total number of atoms. We will effectively invert this nonlinear transformation when the total number of particles N is even.

The finite N Bogoliubov vacuum $|\mathbf{0_b : N}\rangle$. — To write $|0_b\rangle$ in particle representation we need a particle operator $\hat{d}^\dagger$ that commutes with all *quasiparticle* annihilation operators $\hat{b}_m$,

$$
\left[\ \hat{b}_m \ , \ \hat{d}^\dagger \ \right] \ = \ 0 \ , \quad \text{for all } m \ . \qquad (24)
$$

It turns out that a two particle operator of the form

$$
\hat{d} \ = \ \hat{a}_0 \hat{a}_0 \ + \ \sum_{k,l \neq 0} \ Z_{kl} \ \hat{\tilde{a}}_k \hat{\tilde{a}}_l \qquad (25)
$$

is the smallest particle number solution of Eqs.(24). The double summation in the definition of $\hat{d}$ in Eq.(25) runs over an orthonormal basis $\{\tilde{\phi}_1(\vec{x}), \tilde{\phi}_2(\vec{x}), \ldots\}$ in the subspace orthogonal to the condensate wavefunction $\phi_0(\vec{x})$. With the vanishing commutator in Eq.(24) and for an even number of atoms N we can write down Bogoliubov vacuum in the form

$$|0_b : N\rangle \ \propto \ (\hat{d}^\dagger)^{\frac{N}{2}} \ |0\rangle \ , \tag{26}$$

which is annihilated by every $\hat{b}_m$, $\hat{b}_m|0_b : N\rangle = 0$. This particle representation of $|0_b\rangle$ has a finite and well defined number of particles N.

Excited states of the Hamiltonian (19) are created from $|0_b : N\rangle$ by application of the *quasiparticle* creation operators

$$\hat{b}_m^\dagger = \frac{1}{N^{1/2}} \left(\hat{a}_0 \hat{u}_m^\dagger - \hat{a}_0^\dagger \hat{v}_m \right) \ . \tag{27}$$

Equation (26) gives particle representation of the Bogoliubov vacuum for even N. For an odd N there is no N-particle state annihilated by $\hat{b}_m$'s in Eq. (23). This is easy to check for $N = 1$. The ground state of the Bogoliubov Hamiltonian is not annihilated by $\hat{b}_m$'s. This is a direct consequence of the fact that $\hat{b}_m$'s are only approximate bosonic operators: the bosonic commutation relations (18) are fulfilled only approximately when depletion is small. For large N there is no significant difference between N and $N + 1$ so one may apply the results of an even particle system to an odd one. In the following we will illustrate this problem with an exactly solvable example.

Solution for the matrix Z. — To get an explicit $|0_b : N\rangle$ we must solve the condition (24) with respect to Z_{kl}

$$\begin{aligned} 0 \ &= \ \left[\ \hat{b}_m \ , \ \hat{d}^\dagger \ \right] \ = \\ &\left[\frac{1}{N^{1/2}} \left(\hat{a}_0^\dagger \hat{u}_m - \hat{a}_0 \hat{v}_m^\dagger \right), \hat{a}_0^\dagger \hat{a}_0^\dagger + \sum_{k,l \neq 0} Z_{kl} \hat{\tilde{a}}_k^\dagger \hat{\tilde{a}}_l^\dagger \right] = \\ &\frac{\hat{a}_0^\dagger}{N^{1/2}} \left\{ -2\hat{v}_m^\dagger + \sum_{k,l\neq 0} Z_{kl} \left([\hat{u}_m, \hat{\tilde{a}}_k^\dagger] \hat{\tilde{a}}_l^\dagger + [\hat{u}_m, \hat{\tilde{a}}_l^\dagger] \hat{\tilde{a}}_k^\dagger \right) \right\} \ . \end{aligned} \tag{28}$$

It is convenient to define matrices U and V,

$$[\hat{u}_m, \hat{\tilde{a}}_k^\dagger] \ = \ \langle u_m | \tilde{\phi}_k \rangle \ \equiv \ U_{mk} \ , \tag{29}$$

$$\hat{v}_m^\dagger \ \equiv \ V_{mk} \hat{\tilde{a}}_k^\dagger \ . \tag{30}$$

Using the completeness of the basis $\{\tilde{\phi}_1, \tilde{\phi}_2, \ldots\}$ we rewrite the last line of Eq.(28) as a matrix equation

$$V \ = \ U \ Z \ . \tag{31}$$

When u_m's make a complete basis in the subspace orthogonal to ϕ_0, then U_{mk} is an invertible matrix, and we get

$$Z \ = \ U^{-1} \ V \ . \tag{32}$$

The choice of the actual basis $\{\tilde{\phi}_1, \tilde{\phi}_2, \ldots\}$ is in principle arbitrary.

Diagonalization of Z. — We note that the matrix Z introduced in Eq.(25) is symmetric

$$Z \ = \ Z^T \ . \tag{33}$$

Under an additional assumption that Z is real,

$$Z \ = \ Z^* \ , \tag{34}$$

the matrix Z can be diagonalized in an orthonormal eigenbasis $\{\phi_1, \phi_2, \ldots\}$ with real eigenvalues λ_k, and annihilation operators $\{\hat{a}_1, \hat{a}_2, \ldots\}$,

$$\hat{d} \ = \ \hat{a}_0^2 \ + \ \sum_{k\neq 0} \lambda_k \ \hat{a}_k^2 \ . \tag{35}$$

The diagonal $\hat{d}$ gives the finite-N Bogoliubov vacuum in particle representation in the form, see Eq.(26),

$$\begin{aligned} &|0_b : N\rangle \ \sim \ (\hat{d}^\dagger)^{\frac{N}{2}} |0\rangle \ \sim \\ &\sum_{n_0, n_1, \ldots = 0}^{N/2} \qquad \delta_{N, 2n_0 + \ldots + 2n_M} \frac{\sqrt{(2n_0)! \ldots (2n_M)!}}{n_0! \ldots n_M!} \times \\ &\qquad \lambda_1^{n_1} \ldots \lambda_M^{n_M} |2n_0, \ldots, 2n_M\rangle \ . \end{aligned} \tag{36}$$

Here for the sake of convenience we truncate to M Bogoliubov modes. The ket $|2n_0, 2n_1, \ldots, 2n_M\rangle$ is a Fock state with $2n_0, 2n_1, \ldots, 2n_M$ particles in the eigenbasis $\{\phi_0, \phi_1, \ldots, \phi_M\}$. When necessary the particle representation (36) can be translated into an N-particle wavefunction.

As we can see in Eq.(36), every eigenmode can be occupied only by an even number of particles. Particles are depleted from the condensate in pairs ($2n_1 + \ldots + 2n_M$ is even), and every non-condensate eigenmode ϕ_k can be occupied only by an even number of atoms.

Single particle density matrix.— The eigenstates $\{\phi_0, \phi_1, \ldots\}$ of the matrix Z turn out to be also eigenstates of the single particle density matrix,

$$\begin{aligned} &\rho^{(1)}(x, y) \ \equiv \ \langle 0_b : N | \hat{\psi}^\dagger(x) \hat{\psi}(y) | 0_b : N\rangle \ = \\ &\sum_{k=0}^{\infty} \ \langle 0_b : N | \hat{a}_k^\dagger \hat{a}_k | 0_b : N\rangle \ \phi_k^*(x) \phi_k(y) \end{aligned} \tag{37}$$

Off-diagonal elements vanish thanks to the even occupation numbers in the state (36). Eq.(37) provides a familiar interpretation of the eigenmodes $\{\phi_0, \phi_1, \ldots\}$.

The next Section opens our series of examples.

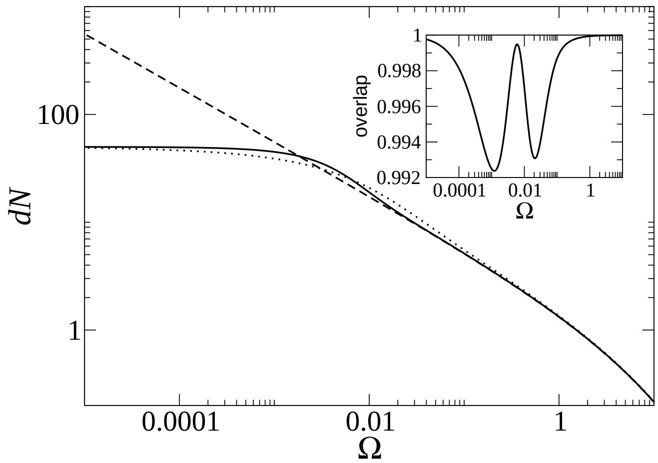

FIG. 1: Number of depleted atoms from a condensate state as a function of frequency Ω [see Eq. (38)]. The solid line corresponds to the exact results, the dashed line to Eq. (49), while the dotted line is depletion calculated directly from the Bogoliubov eigenstate in the particle representation, Eq. (53). The inset shows the overlap of the exact state and the Bogoliubov state $|0_b : N\rangle$, Eq. (52), as a function of Ω. Data for the double well system with $N = 100$ atoms. $\Omega \approx 0.01$ is the crossover point between the Mott insulator and superfluid.

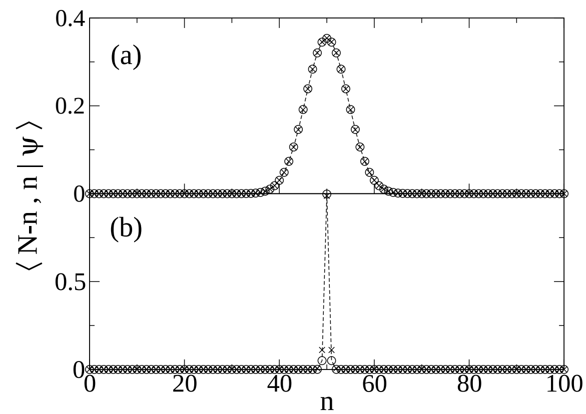

FIG. 2: Ground state $|\psi\rangle$ of a condensate in a double well potential for $N = 100$ atoms and for $\Omega = 10$ (a), $\Omega = 0.001$ (b). Circles (connected with a dashed line) correspond to the exact results while crosses are related to the Bogoliubov eigenstates in the particle representation. The ground states $|\psi\rangle$ are projected on Fock states $|N-n, n\rangle$ where $N-n$ is a number of atoms in the left well and n is a number of atoms in the right well.

IV. DOUBLE WELL

Let us put N atoms in a double well potential. In the tight binding approximation, when we restrict only to the Hilbert space spanned by the ground states in each well, this system is described by a boson Hubbard model

$$H_{2\mathrm{W}} \;=\; -\;\Omega\;\left(\;\hat{c}_1^\dagger \hat{c}_2 \;+\; \hat{c}_2^\dagger \hat{c}_1\;\right) \;+\; \frac{1}{2}\sum_{j=1,2} \hat{n}_j(\hat{n}_j - 1)\;. \tag{38}$$

Here $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ for $j = 1, 2$ is an operator of the number of atoms in the j-th well. The $\hat{n}_j(\hat{n}_j - 1)$ terms describe repulsive interactions between atoms in each well. The first term in the Hamiltonian is responsible for tunneling between different wells. All units were rescaled so that the only dimensionless parameter is the tunneling rate Ω.

On the level of the GPE this system is described by a condensate wavefunction which is a vector of two complex amplitudes,

$$\phi_0 \;=\; (\;\phi_{0,1}\;,\;\phi_{0,2}\;)\;, \tag{39}$$

one amplitude for each well. Solution of the GPE for the ground state results in a symmetric state

$$\phi_0 \;=\; \frac{1}{\sqrt{2}}\;(\;1\;,\;1\;)\;. \tag{40}$$

Atoms in this condensate are annihilated by

$$\hat{a}_0 \;=\; \frac{\hat{c}_1 + \hat{c}_2}{\sqrt{2}}\;. \tag{41}$$

The only mode orthogonal to ϕ_0 is

$$\phi_1 \;=\; \frac{1}{\sqrt{2}}\;(\;1\;,\;-1\;)\;, \tag{42}$$

with an annihilation operator

$$\hat{a}_1 \;=\; \frac{\hat{c}_1 - \hat{c}_2}{\sqrt{2}}\;. \tag{43}$$

The double well system has been studied theoretically [13] and its multiwell generalizations were a subject of recent experiments [4]. The ground state properties of this system are well known. In the regime of $\Omega \gg N$ the ground state is a quasi-coherent state

$$\left(\hat{c}_1^\dagger + \hat{c}_2^\dagger\right)^N |0\rangle \;\sim\; \left(\hat{a}_0^\dagger\right)^N |0\rangle\;, \tag{44}$$

where all N atoms are in the same condensate wavefunction (40) and the number of depleted atoms $N_1 = \langle \hat{a}_1^\dagger \hat{a}_1 \rangle$ is zero.

In the Mott insulator regime of $N\Omega \ll 1$ the ground state is a Mott insulator,

$$\left(\hat{c}_1^\dagger\right)^{\frac{N}{2}} \left(\hat{c}_2^\dagger\right)^{\frac{N}{2}} |0\rangle\;. \tag{45}$$

This state is very far from the condensate (44), it has a huge fraction of depleted atoms $\frac{\langle \hat{c}_1^\dagger \hat{c}_1 \rangle}{N} = \frac{1}{2}$. One half of all atoms are depleted from the condensate wavefunction (40) predicted by the GPE.

Quasiparticle representation. — The Hubbard model (38) has been studied in the framework of the BT only very recently [14]. The Bogoliubov-de Gennes equations are

$$
\begin{aligned}
-\Omega(u_2 - u_1) + \frac{N}{2}(u_1 + v_1) &= +\omega u_1 \ , \\
-\Omega(u_1 - u_2) + \frac{N}{2}(u_2 + v_2) &= +\omega u_2 \ , \\
-\Omega(v_2 - v_1) + \frac{N}{2}(v_1 + u_1) &= -\omega v_1 \ , \\
-\Omega(v_1 - v_2) + \frac{N}{2}(v_2 + u_2) &= -\omega v_2 \ , \qquad (46)
\end{aligned}
$$

The index $j = 1, 2$ in u_j and v_j numbers a well. These equations give only one Bogoliubov mode orthogonal to the condensate ϕ_0

$$
u \ = \ \frac{X}{\sqrt{X^2 - 1}} \, \phi_1 \ , \quad v \ = \ \frac{-1}{\sqrt{X^2 - 1}} \, \phi_1 \ , \qquad (47)
$$

where

$$
X \ = \ \left(1 + \frac{4\Omega}{N}\right) + \sqrt{\left(1 + \frac{4\Omega}{N}\right)^2 - 1} \ . \qquad (48)
$$

In the *quasiparticle* representation the number of depleted atoms in the Bogoliubov vacuum state is *approximately* given by [8]

$$
\begin{aligned}
dN \ &= \ \int dx \ \delta\hat{\psi}^\dagger \delta\hat{\psi} \ \approx \ \int dx \ \delta\hat{\psi}^\dagger \hat{a}_0 \frac{1}{N} \hat{a}_0^\dagger \delta\hat{\psi} \\
&= \int dx \ \hat{\Lambda}^\dagger \hat{\Lambda} \ \ = \ \langle v|v \rangle \ = \ \frac{1}{X^2 - 1} \ . \qquad (49)
\end{aligned}
$$

The approximate equality is justified when the depletion is small and $N \gg 1$. This dN is plotted with a dashed line in Fig.1. When $\Omega \to 0$, then the dN diverges like $dN \sim \Omega^{-1/2}$. As N is finite, the divergence in dN is unphysical. The divergence of dN is not present when we calculate depletion directly from the Bogoliubov state in the particle representation.

Particle representation. — The operator $\hat{b}$ for the Bogoliubov mode (47) is

$$
\hat{b} = \langle u|\Lambda \rangle - \langle v|\Lambda^\dagger \rangle = \frac{X \hat{a}_0^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_0}{\sqrt{N(X^2 - 1)}} \ . \qquad (50)
$$

We look for a two-atom annihilation operator $\hat{d} \sim \hat{a}_0^2 + \lambda_1 \hat{a}_1^2$ such that $\hat{b}$ commutes with $\hat{d}^\dagger$, $[\hat{b}, \hat{d}^\dagger] = 0$. The solution is

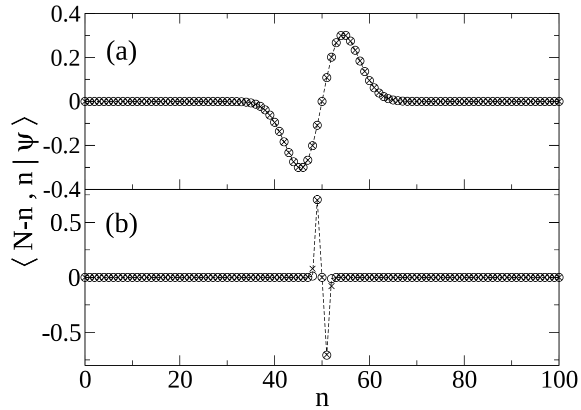

FIG. 3: The first excited state $|\psi\rangle$ of a condensate in a double well potential for $N = 100$ atoms and for $\Omega = 10$ (a), $\Omega = 0.001$ (b). Circles (connected with a dashed line) correspond to the exact results while crosses are related to the Bogoliubov eigenstate with one quasiparticle $\hat{b}^\dagger |0_b : N\rangle$. The states $|\psi\rangle$ are projected on $|N - n, n\rangle$ states where $N - n$ is a number of atoms in the left well and n is a number of atoms in the right one.

$$
\hat{d} \sim \hat{a}_0^2 - \frac{\hat{a}_1^2}{X} \ . \qquad (51)
$$

This operator defines the Bogoliubov vacuum in the particle representation

$$
|0_b : N\rangle \sim \left(\hat{d}^\dagger\right)^{\frac{N}{2}} |0\rangle \ . \qquad (52)
$$

The number of depleted atoms in this state,

$$
dN = \langle 0_b : N | \hat{a}_1^\dagger \hat{a}_1 | 0_b : N \rangle \qquad (53)
$$

is plotted with a dotted line in Fig.1. It compares surprisingly well with dN in the exact ground state (solid line) even in the Mott insulator regime ($N\Omega \ll 1$). In contrast, in the insulator regime the standard Bogoliubov theory (dashed line) gives an unphysically divergent dN.

In Fig. 2 we compare the Bogoliubov eigenstates with the exact ones in both weak and strong tunneling regimes. We find surprising agreement between both solutions that is present even in the Mott insulator regime. To see how the Bogoliubov vacuum smoothly interpolates between the quasi-coherent state (44) for large Ω (large X), and the Mott insulator (45) for small Ω ($X \to 1$) it is convenient to rewrite Eq.(51) as a product of annihilation operators in two in general non-orthogonal modes,

$$
d \ \sim \ \left(\hat{a}_0 + \frac{\hat{a}_1}{\sqrt{X}}\right) \left(\hat{a}_0 - \frac{\hat{a}_1}{\sqrt{X}}\right) \ . \qquad (54)
$$

With this d the Bogoliubov vacuum becomes a quasi-Fock state

$$|0_b : N\rangle \ \sim \ \left(\hat{a}_0^\dagger + \frac{\hat{a}_1^\dagger}{\sqrt{X}}\right)^{\frac{N}{2}} \left(\hat{a}_0^\dagger - \frac{\hat{a}_1^\dagger}{\sqrt{X}}\right)^{\frac{N}{2}} \ |0\rangle \ . \quad (55)$$

The two modes become the same for large Ω (large X), and they become orthogonal for $\Omega \to 0$ ($X \to 1$). This quasi-Fock representation may be useful in any case when one can approximately truncate the Hilbert space to only one Bogoliubov mode. For the double well this truncation is exact.

In Fig. 3 we compare the first excited state of the double well system with the Bogoliubov eigenstate with one quasiparticle $\hat{b}^\dagger|0_b : N\rangle$ for two values of Ω, one in the Mott insulator and the other in the superfluid regime. Like for the ground state we find surprisingly good agreement between the two states even in the Mott regime.

The surprising agreement between the Bogoliubov eigenstates and the exact eigenstates that we found even in the Mott insulator regime is rather an exception than a rule, as we show for a triple well system.

V. PERIODIC TRIPLE WELL

The Bogoliubov theory applied to the double well potential turns out to be surprisingly good. In the present example it does not work so well and we can investigate how the Bogoliubov approximation stops working with increasing depletion from the condensate. The periodic triple well system is described by a boson Hubbard Hamiltonian

$$H_{3\mathrm{W}} \ = \ - \ \Omega \sum_{\langle i,j\rangle} \hat{c}_i^\dagger \hat{c}_j \ + \ \frac{1}{2}\sum_{j=1}^{3} \ \hat{n}_j(\hat{n}_j - 1) \ . \quad (56)$$

We proceed similarly as for the double well. The ground state of the GPE is

$$\phi_0 = \frac{1}{\sqrt{3}}\,(1,1,1) \quad (57)$$

and it is associated with an annihilation operator $\hat{a}_0$. There are two modes orthogonal to ϕ_0

$$\phi_+ = \frac{1}{\sqrt{3}}\left(1, e^{+\frac{2\pi i}{3}}, e^{-\frac{2\pi i}{3}}\right) \ ,$$
$$\phi_- = \frac{1}{\sqrt{3}}\left(1, e^{-\frac{2\pi i}{3}}, e^{+\frac{2\pi i}{3}}\right) \quad (58)$$

with annihilation operators $\hat{a}_+$ and $\hat{a}_-$ respectively. The Bogoliubov-de Gennes equations give two Bogoliubov modes, let us call them $+$ and $-$, with

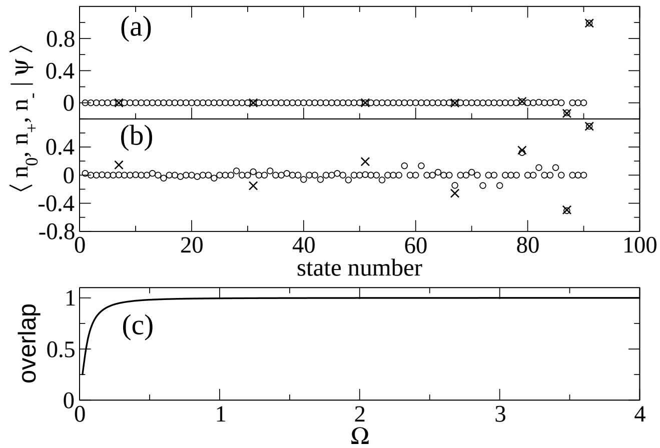

FIG. 4: Ground state of a condensate in a triple well potential for $N = 12$ atoms and for $\Omega = 4$ (a), $\Omega = 0.1$ (b). Circles correspond to the exact results while crosses to the Bogoliubov eigenstates in the particle representation. The states $|\psi\rangle$ are projected on $|n_0, n_+, n_-\rangle$ states where n_0 is a number of atoms in a condensate wavefunction Eq. (57) while n_+ and n_- correspond to numbers of atoms in the orthogonal modes ϕ_+ and ϕ_- Eq. (58). If the depletion is small (in (a) $dN \approx 0.03$) the Bogoliubov eigenstates match well the exact ones. However, for a large depletion (in (b) $dN \approx 1.9$ that is significant as compared to $N = 12$) the exact states become considerably different from the Bogoliubov prediction that only states $|N-2i, i, i\rangle$ should give nonzero contributions. Panel (c) shows the overlap of the exact and Bogoliubov eigenstates as a function of Ω for $\Omega \in [0.02, 4]$.

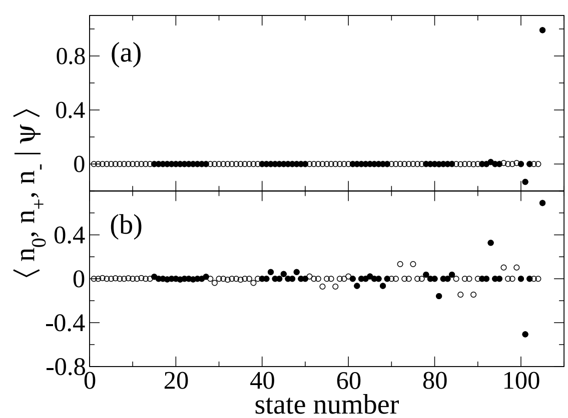

FIG. 5: Exact ground state of a condensate in a triple well potential for $N = 13$ atoms and for $\Omega = 4$ (a), $\Omega = 0.1$ (b). The states $|\psi\rangle$ are projected on $|n_0, n_+, n_-\rangle$ states where n_0 is a number of atoms in a condensate wavefunction Eq. (57) while n_+ and n_- correspond to numbers of atoms in the orthogonal modes ϕ_+ and ϕ_- Eq. (58). Contributions of states that correspond to even numbers of depleted atoms from the condensate, i.e. $|N-2i, \ldots, \ldots\rangle$, are marked by full circles. Compare the structure of the eigenstates with the similar results for $N = 12$ presented in Fig. 4.

$$u_{\pm} = \frac{X\phi_{\pm}}{\sqrt{X^2-1}} \ , \quad v_{\pm} = \frac{-\phi_{\pm}}{\sqrt{X^2-1}} \ , \tag{59}$$

where

$$X = \left(1+\frac{9\Omega}{N}\right) + \sqrt{\left(1+\frac{9\Omega}{N}\right)^2 - 1} \ . \tag{60}$$

These modes give

$$\hat{b}_{\pm} = \frac{X\hat{a}_0^\dagger \hat{a}_{\pm} + \hat{a}_0 \hat{a}_{\mp}^\dagger}{\sqrt{N(X^2-1)}} \ . \tag{61}$$

The operators $\hat{b}_{\pm}$ commute with a $\hat{d}^\dagger$ such that

$$\hat{d} = \hat{a}_0\hat{a}_0 - \frac{2}{X}\hat{a}_+\hat{a}_- \ , \tag{62}$$

which can be easily diagonalized by operators

$$\hat{a}_1 = \frac{\hat{a}_+ + \hat{a}_-}{\sqrt{2}} \ , \quad \hat{a}_2 = \frac{\hat{a}_+ - \hat{a}_-}{\sqrt{2}} \ , \tag{63}$$

with eigenvalues

$$\lambda_1 \ = \ -\lambda_2 \ = \ -\frac{1}{X} \ . \tag{64}$$

In the Bogoliubov theory only pairs of atoms are depleted from a condensate wavefunction. Recently, in exact stochastic calculations Carusotto and Castin [15] also observed such a pairwise depletion from a condensate in a harmonic trap. In Fig. 4a we show the structure of a Bogoliubov vacuum together with the exact ground state of the triple well system which confirms the predicted pairwise depletion. However, with decreasing tunneling rate Ω, that makes the interaction between atoms relatively stronger, the exact ground state looses the pairwise structure expected in the linear Bogoliubov theory, see Fig. 4b. This is a clear signature of a breakdown of the linearized Bogoliubov theory.

In Fig. 5 we show an exact ground state for an odd number of particles. Again like for even N particles are depleted in pairs. Although we were not able to find any simple form for the Bogoliubov ground state with odd N, this example suggest that, especially for large N, accurate predictions can be extrapolated from even N.

VI. BOSE-EINSTEIN CONDENSATE IN A HARMONIC TRAP

In the previous two exactly solvable examples the construction of the finite N Bogoliubov vacuum was relatively easy because there were only one or two Bogoliubov modes. In this Section we analyze the finite N Bogoliubov vacuum for ground and solitonic states of a condensate in a 1D harmonic trap

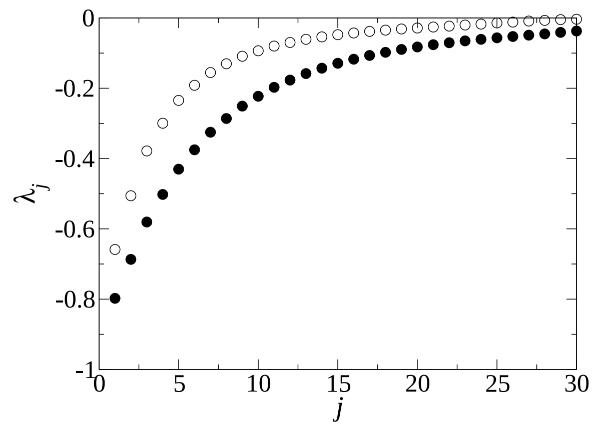

FIG. 6: Eigenvalues λ_j of Z matrix corresponding to the ground state of a condensate in a 1D harmonic trap for $gN = 20$ (open circles) and $gN = 50$ (full circles). Note that with increasing gN more and more modes get significant contributions to a condensate eigenstate, see Eq. (36).

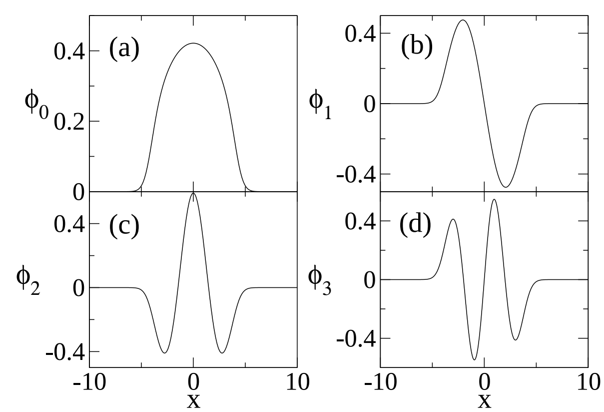

FIG. 7: Plots of a condensate mode $\phi_0(x)$ and three the most significant eigenmodes $\phi_j(x)$ to which the condensate is depleted for the system in a ground state of a 1D harmonic trap for $gN = 50$. Note that $\phi_j(x)$'s are eigenmodes of $\rho^{(1)}(x,y)$, compare Eq.(37).

$$V(x) \ = \ \frac{1}{2}x^2 \ . \tag{65}$$

The solitonic state is the first excited antisymmetric state of the GPE [2].

We constructed the Bogoliubov vacuum in particle representation in the following steps. To begin with we found the relevant stationary state ϕ_0 of the GPE in

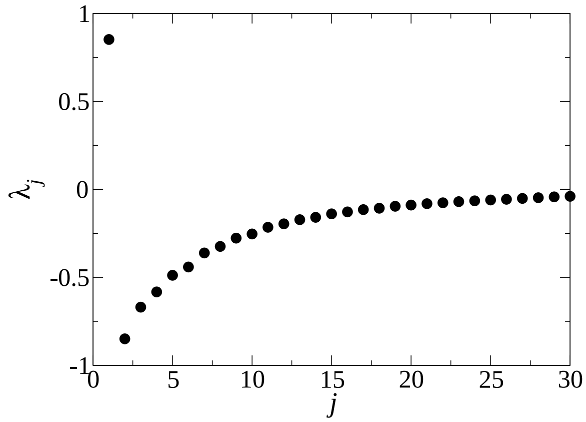

FIG. 8: Eigenvalues λ_j of Z matrix corresponding to a solitonic state of a condensate in a 1D harmonic trap for $gN = 50$. Compare the present plot with the results for a condensate in a ground state presented in Fig. 6.

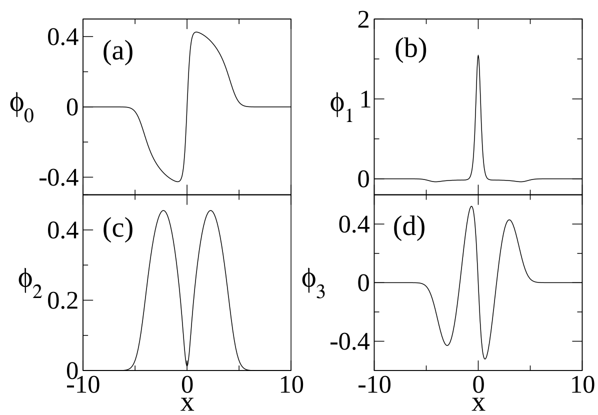

FIG. 9: Plots of a condensate mode $\phi_0(x)$ and three the most significant modes $\phi_j(x)$ to which the condensate is depleted for the system in a solitonic state of a 1D harmonic trap for $gN = 50$. Note that $\phi_j(x)$'s are eigenmodes of $\rho^{(1)}(x, y)$, compare Eq.(37).

a harmonic potential: the ground state or the solitonic state. Then we diagonalized the Bogoliubov-de Gennes equations (14) for a given background ϕ_0 and projected the obtained modes on the subspace orthogonal to the condensate wavefunction like in Eq.(15). In this way we obtained the u_j and v_j modes of the number-conserving Bogoliubov theory. In the next step we constructed matrices U and V like in Eqs.(29,30). In order to construct such matrices we had to choose a basis in the subspace orthogonal to the condensate wavefunction ϕ_0. To make the matrices finite we had to truncate the number of Bogoliubov modes to a finite M. We got fast convergence of results with increasing M for a basis constructed out of the u_j modes,

$$\begin{aligned} \tilde{\phi}_1 &\sim u_1 \ , \\ \tilde{\phi}_2 &\sim u_2 - \tilde{\phi}_1 \langle \tilde{\phi}_1 | u_2 \rangle \ , \ \dots \ . \end{aligned} \tag{66}$$

Finally, we solved Eq. (31) with respect to Z and then diagonalized the obtained Z matrix. The eigenvalues were ordered with decreasing modulus, $|\lambda_1| > |\lambda_2| > \ldots > |\lambda_M|$. As is clear from the state (36), even a small decrease of $|\lambda_k|$ from one mode to the next results in a substantial drop in the average number of atoms occupying this mode.

In Fig. 6 we plot the spectrum of the Z matrix, corresponding to the ground state of the condensate in a harmonic trap for two different interaction strengths gN. With increasing gN more and more modes have significant contribution to the condensate eigenstate. Because pairs of atoms are depleted from the condensate, the single particle eigenmodes ϕ_k are allowed to be both even and odd as shown in Fig. 7. Note that ϕ_j are also eigenmodes of the single particle density matrix, see Eq.(37).

For a condensate in a solitonic state, in the spectrum of the Z matrix (Fig. 8) the dominant eigenvalue λ_1 is positive (contrary to other eigenvalues) and the corresponding anomalous mode is localized in the soliton notch [16], see Fig. 9. The anomalous mode $\phi_1(x)$ is a (nearly) zero mode related to translational motion of the dark soliton with respect to the condensate.

VII. CONCLUSION

In the present paper we have constructed the Bogoliubov eigenstates in the particle representation. The particle representation gives much more intuitive insight into physical processes that are responsible for depletion of a condensate. Comparison of the derived eigenstates with exact solutions for model systems reveals that as far as a number of depleted atoms is small the Bogoliubov eigenstates match well exact eigenstates. In the Bogoliubov theory the condensate is depleted by pairs of atoms. However, when strength of the interaction between atoms increases the linear Bogoliubov theory breaks down and the condensate starts being depleted by odd numbers of particles.

We have applied our approach to analyze structure of a realistic condensate in the ground and solitonic states of a harmonic trap. Having calculated eigenstates in the particle representation one can in principle extract any information about a system and simulate results of any measurement. Examples of such realistic applications will be given in our future publication [17].

Acknowledgments

Support of KBN under projects 2 P03B 092 23 (J.D.), and 5 P03B 088 21 (K.S.) is acknowledged.

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